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Uncertainty Quantification and Data Fusion

Royset, Johannes

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Uncertainty Quantification and Data Fusion

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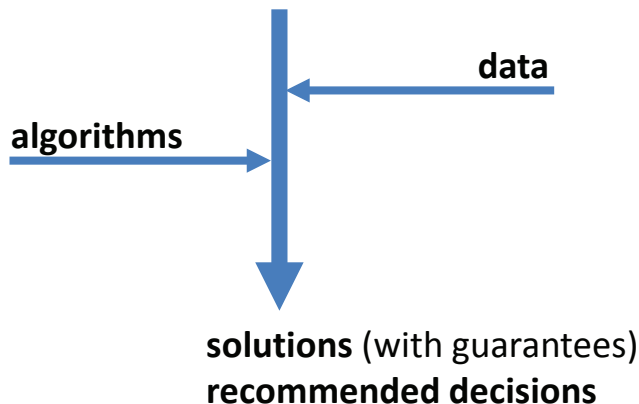
ICSP Tutorial, Bergamo, July 2013

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Components of **deterministic** optimization practice

modeling

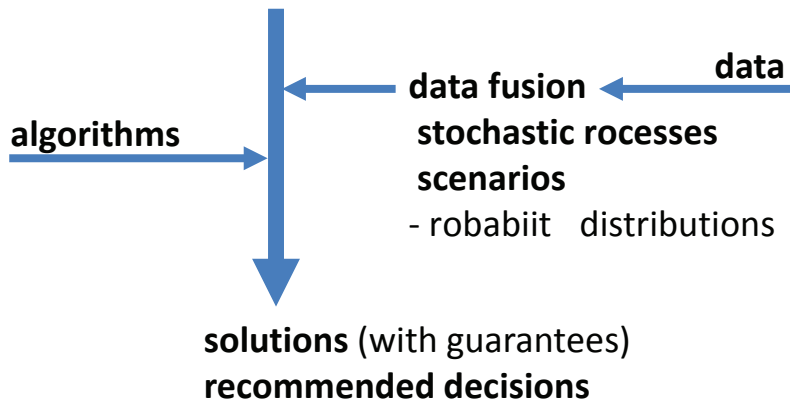
- objective function
- constraints



Components of stochastic optimization practice

modeling

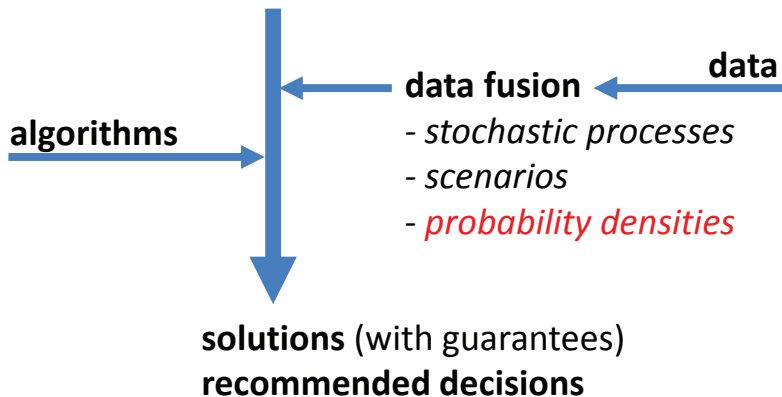
- objective and constraint functions
- decision stages uncertain code



Components of stochastic optimization practice

modeling

- objective and constraint functions
- *decision stages, uncertainty model*

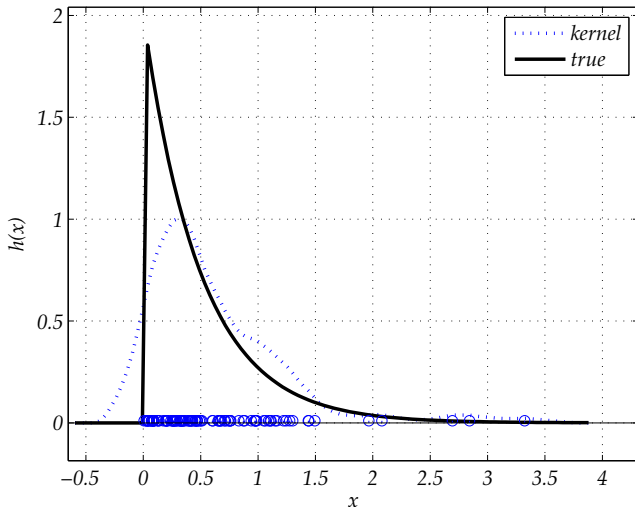


Example: 100 observations of demand

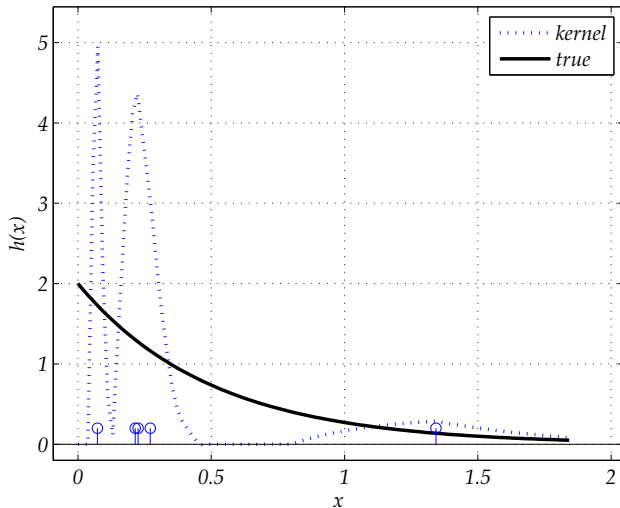
Possibilities: Use the 100 scenarios; fit to assumed parametric form; Bayesian update; nonparametric estimation

Example: 100 observations of demand

Possibilities: Use the 100 scenarios; fit to assumed parametric form; Bayesian update; nonparametric estimation



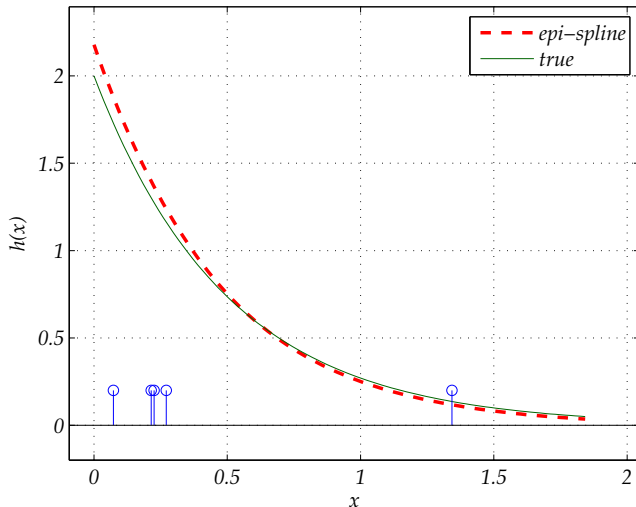
...but with only 5 observations



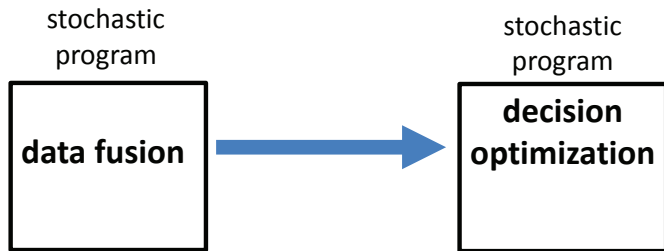
Almost always **soft information** available

Use stochastic programming!

Same 5 points, but with epi-splines and soft info. (nonnegativity, continuous differentiable, and decreasing)



Two roles for stochastic programming



Independent value in data fusion and uncertainty quant.

Engineering, biological, physical systems

- ▶ Input: random V (“known” distribution)
- ▶ System function G ; implicitly defined e.g. by simulation
- ▶ Output: random variable

$$X = G(V)$$

Independent value in data fusion and uncertainty quant.

Engineering, biological, physical systems

- ▶ Input: random V (“known” distribution)
- ▶ System function G ; implicitly defined e.g. by simulation
- ▶ Output: random variable

$$X = G(V)$$

Given observations (data) $x^1 = G(v^1), \dots, x^\nu = G(v^\nu)$, we seek a description of X :

- ▶ mean, standard deviation
- ▶ quantile, superquantile
- ▶ distribution, density (pdf)

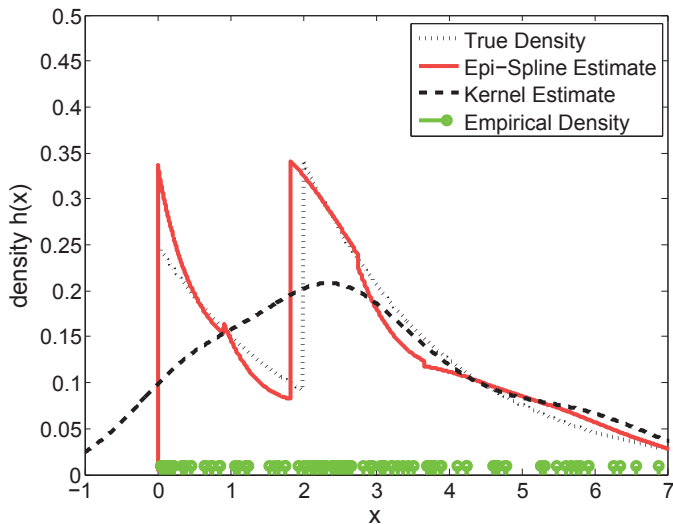
Main challenge: few data points; little relevant data

But **soft information** might be available

Example: M/M/1; 50% of customers delayed for fixed time

X = customer time-in-service; 100 observations

Soft info: Isc , $X \geq 0$, pointwise Fisher, unimodal upper tail



Outline

- ▶ Density estimation as a stochastic program
- ▶ Epi-splines: pliable approximation tools
- ▶ Consistency and asymptotics
- ▶ Fusion of hard and soft information
- ▶ Numerical examples

Formulation of density estimation problem

Kullback-Leibler divergence from density h to density g on \mathbf{R}

$$d_{KL}(h||g) = \int_{-\infty}^{\infty} h(x) \log \frac{h(x)}{g(x)} dx$$

Facts:

$$d_{KL}(h||g) \geq 0 \text{ for all densities } h, g$$

$$d_{KL}(h||g) = 0 \iff h(x) = g(x) \text{ (Lebesgue) almost every } x \in \mathbf{R}$$

Formulation (cont.)

Consequently, for density $h^0 \in \mathcal{H}$:

If

$$\begin{aligned} \tilde{h} &\in \operatorname{argmin}_h d_{KL}(h^0 || h) \\ \text{s.t.} \quad &\int_{-\infty}^{\infty} h(x) dx = 1 \\ &h \geq 0 \\ &h \in \mathcal{H} \end{aligned}$$

then

$$\tilde{h} = h^0 \text{ a.e.}$$

Formulation (cont.)

Let X^0 be a random variable with density h^0

Then,

$$d_{KL}(h^0||h) = \int_{-\infty}^{\infty} h^0(x) \log \frac{h^0(x)}{h(x)} dx = E\{\log h^0(X^0)\} - E\{\log h(X^0)\}$$

Formulation (cont.)

Let X^0 be a random variable with density h^0

Then,

$$d_{KL}(h^0||h) = \int_{-\infty}^{\infty} h^0(x) \log \frac{h^0(x)}{h(x)} dx = E\{\log h^0(X^0)\} - E\{\log h(X^0)\}$$

So minimizing $d_{KL}(h^0||h)$ is equivalent to

$$\tilde{h} \in \operatorname{argmax}_h E\{\log h(X^0)\}$$

$$\text{s.t.} \quad \int_{-\infty}^{\infty} h(x) dx = 1$$

$$h \geq 0, \quad h \in \mathcal{H}$$

Of course, expectation is with respect to the **true** distribution

Formulation (cont.)

Data (sample) X^1, X^2, \dots, X^ν available

$$\begin{aligned} h^\nu \in \operatorname{argmax}_h \frac{1}{\nu} \sum_{i=1}^{\nu} \log h(X^i) &= \log \left(\prod_{i=1}^{\nu} h(X^i) \right)^{1/\nu} \\ \text{s.t.} \quad \int_{-\infty}^{\infty} h(x) dx &= 1 \\ h &\geq 0, h \in \mathcal{H} \end{aligned}$$

Formulation (cont.)

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approximates

$$\begin{aligned} \tilde{h} \in \operatorname{argmax}_h E\{\log h(X^0)\} \\ \text{s.t.} \quad \int_{-\infty}^{\infty} h(x) dx &= 1 \\ h &\geq 0, h \in \mathcal{H} \end{aligned}$$

Approximation is a **max log-likelihood problem**

Incorporating soft information

$$\begin{aligned} h^\nu \in \operatorname{argmax}_h \frac{1}{\nu} \sum_{i=1}^{\nu} \log h(X^i) &= \log \left(\prod_{i=1}^{\nu} h(X^i) \right)^{1/\nu} \\ \text{s.t.} \quad \int_{-\infty}^{\infty} h(x) dx &= 1 \\ h &\geq 0, h \in H^\nu \subset \mathcal{H} \end{aligned}$$

where H^ν includes essentially **any soft information** about h^0 :

- ▶ support bounds
- ▶ density continuity, smoothness
- ▶ density shape (unimodal, decreasing, etc.)
- ▶ moments
- ▶ proximity to known density
- ▶ system knowledge (convex G , gradient of G)

Outline

- ▶ Density estimation as a stochastic program
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Challenge: infinite-dimensional problems

$$\begin{aligned} h^\nu \in \operatorname{argmax}_h \frac{1}{\nu} \sum_{i=1}^{\nu} \log h(X^i) &= \log \left(\prod_{i=1}^{\nu} h(X^i) \right)^{1/\nu} \\ \text{s.t.} \quad \int_{-\infty}^{\infty} h(x) dx &= 1 \\ h &\geq 0, \quad h \in H^\nu \subset \mathcal{H} \end{aligned}$$

Need approximation of \mathcal{H} by set of **flexible** functions given by **finite** number of parameters

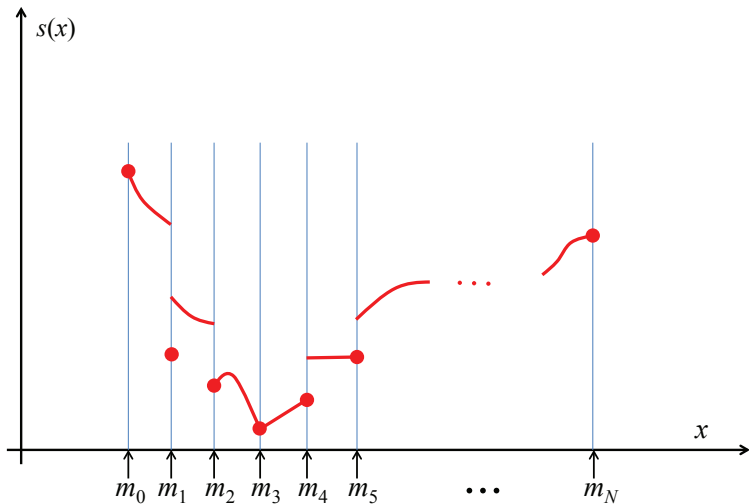
Exponential epi-spline estimator

Given sample X^1, \dots, X^ν , the **exponential epi-spline** estimator of the true density is

$$h^\nu = e^{-s^\nu},$$

where s^ν is an **epi-spline**

Epi-splines: piecewise polynomial functions



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where s^ν is an **epi-spline**

Main features:

- ▶ finite number of parameters; powerful optimization technology available
- ▶ approximates to arbitrary accuracy essentially any function
- ▶ easily includes soft information
- ▶ substantially more flexible and pliable than 'classical' splines
- ▶ nonnegativity achieved automatically

Epi-splines

- ▶ *Number of partitions N*
- ▶ *Mesh $m = \{m_k\}_{k=0}^N$, where $m_{k-1} < m_k$, $k = 1, 2, \dots, N$*
- ▶ *Estimation on $[m_0, m_N]$*
- ▶ *Order p*

Epi-splines

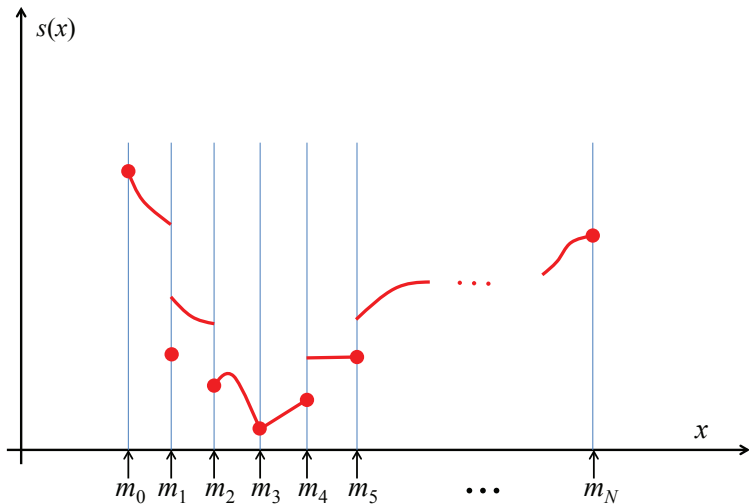
- ▶ *Number of partitions* N
- ▶ *Mesh* $m = \{m_k\}_{k=0}^N$, where $m_{k-1} < m_k$, $k = 1, 2, \dots, N$
- ▶ *Estimation on* $[m_0, m_N]$
- ▶ *Order* p

Definition

$\text{e-spl}^p(m)$ = family of (basic) epi-splines of order p , with mesh $m = \{m_k\}_{k=0}^N$, consists of:

- ▶ functions $s : [m_0, m_N] \rightarrow \mathbb{R}$
- ▶ that are polynomials of degree p in each segment (m_{k-1}, m_k) , $k = 1, 2, \dots, N$, and
- ▶ that are finite valued at m_0, m_1, \dots, m_N

Representation of epi-spline



Representation of epi-spline

Every $s \in \text{e-spl}^p(m)$, with $m = \{m_k\}_{k=0}^N$, is uniquely represented by

$$r = (s_0, s_1, \dots, s_N, a_1, a_2, \dots, a_N), \quad s_k \in \mathbf{R}, \quad a_k \in \mathbf{R}^{p+1},$$

such that

$$s(x) = \langle c(x), r \rangle, \quad x \in [m_0, m_N],$$

where

$$c(x) = \begin{cases} (0, \dots, 0, 1, x - m_{k-1}, \dots, (x - m_{k-1})^p, 0, \dots, 0) & \text{if } x \in (m_{k-1}, m_k), k = 1, \dots, N \\ (0, \dots, 0, 1, 0, \dots, 0) & \text{if } x = m_k, k = 0, 1, \dots, N. \end{cases}$$

Approximation of functions by epi-splines

$\text{lsc-fcns}([l, u]) =$

lower semicontinuous functions (lsc) on $[l, u]$ not $\equiv \infty$

Adopt metric topology induced by the epi-distance

Approximation of functions by epi-splines

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lower semicontinuous functions (lsc) on $[l, u]$ not $\equiv \infty$

Adopt metric topology induced by the epi-distance

Need to allow for

- ▶ jumps (discontinuous densities)
- ▶ infinity (due to e^{-s})
- ▶ pointwise constraints (soft information)
- ▶ mixtures with probability mass functions
- ▶ subsequent maximization of densities (find modes)

Epi-distance

point-to-set distance = $d(x, S) = \inf_{y \in S} \|x - y\|$ for $S \subset \mathbf{R}^2$

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epi-graph of $f = \text{epi } f = \{(x, \beta) \in \mathbf{R}^2 \mid f(x) \leq \beta\}$

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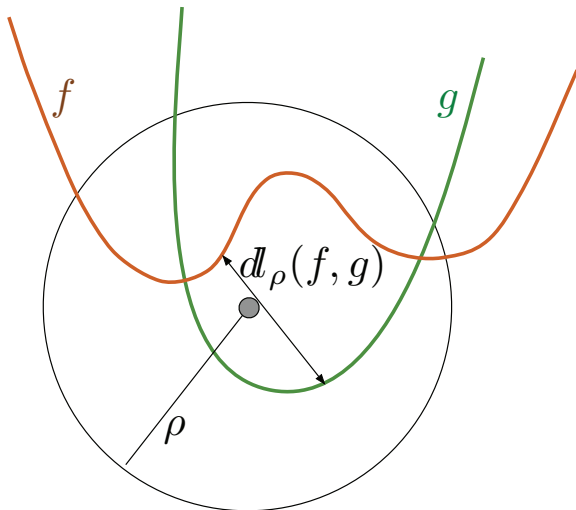
$$\text{Epi-distance} = dl(f, g) = \int_0^\infty dl_\rho(f, g) e^{-\rho} d\rho$$

where for $\rho \geq 0$

$$dl_\rho(f, g) = \max_{\|x\| \leq \rho} |d(x, \text{epi } f) - d(x, \text{epi } g)|$$

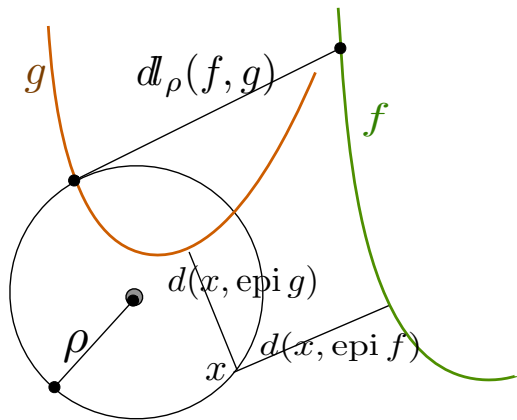
Epi-distance (cont.)

$$dl_{\rho}(f, g) = \max_{\|x\| \leq \rho} |d(x, \text{epi } f) - d(x, \text{epi } g)|$$



Epi-distance (cont.)

$$dl_{\rho}(f, g) = \max_{\|x\| \leq \rho} |d(x, \text{epi } f) - d(x, \text{epi } g)|$$



Characterization of convergence

For any $\bar{\rho} \geq 0$:

$$dl(f^\nu, f) \rightarrow 0 \iff dl_\rho(f^\nu, f) \rightarrow 0 \text{ for all } \rho \geq \bar{\rho}$$

$(\text{lsc-fcns}([l, u]), dl)$ complete separable metric space

Convergence of exponential epi-splines

exponential epi-splines $= \text{x-spl}^p(m) = \{e^{-s} \mid s \in \text{e-spl}^p(m)\}$

hypo-distance $dl_{\text{hypo}}(f, g) = dl(-f, -g)$

$h^\nu, h^0 \in \text{x-spl}^p(m)$, $h^\nu = e^{-s^\nu} = e^{-\langle c(\cdot), r^\nu \rangle}$, $h^0 = e^{-s^0} = e^{-\langle c(\cdot), r^0 \rangle}$

Then, the following hold:

$$r^\nu \rightarrow r^0 \iff h^\nu \rightarrow h^0 \text{ uniformly on } [m_0, m_N]$$

$$\implies dl_{\text{hypo}}(h^\nu, h^0) \rightarrow 0 \iff dl(s^\nu, s^0) \rightarrow 0$$

Moreover, if h^ν, h^0 are usc, then also

$$h^\nu \rightarrow h^0 \text{ uniformly on } [m_0, m_N] \iff dl_{\text{hypo}}(h^\nu, h^0) \rightarrow 0$$

Properties of (exponential) epi-splines

If $\{m^\nu\}_{\nu=1}^\infty$ are refining meshes, then

- ▶ $\text{lsc } \{e\text{-spl}^p(m^\nu)\}_{\nu=1}^\infty$ dense in $\text{lsc-fcns}([l, u])$
- ▶ $\text{usc } \{x\text{-spl}^p(m^\nu)\}_{\nu=1}^\infty$ dense in $\{e^{-s} \mid s \in \text{lsc-fcns}([l, u])\}$

Examples

- ▶ most densities approximated to arbitrary accuracy

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Examples

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- ▶ normal density represented by $\text{e-spl}^2(m)$ on $[m_0, m_N]$ for any m
- ▶ exponential density represented by $\text{e-spl}^1(m)$ on $[m_0, m_N]$ for any choice of m with $m_0 = 0$
- ▶ lognormal and Pareto also exactly represented after transformation

Recall: maximize log-likelihood

$$\begin{aligned} h^\nu &\in \operatorname{argmax}_h \frac{1}{\nu} \sum_{i=1}^{\nu} \log h(X^i) \\ \text{s.t.} \quad &\int_{-\infty}^{\infty} h(x) dx = 1 \\ &h \geq 0 \\ &h \in H^\nu \subset \mathcal{H} \end{aligned}$$

Now $h = e^{-\langle c(\cdot), r \rangle}$ and optimize over $r \in \mathbb{R}^{(p+2)N+1}$ instead

Resulting optimization problem

$$\begin{aligned} \min_r \quad & \frac{1}{\nu} \sum_{i=1}^{\nu} \langle c(X^i), r \rangle \\ \text{s.t.} \quad & \int_{m_0}^{m_N} e^{-\langle c(x), r \rangle} dx = 1 \\ & r \in R^{\nu} = \left\{ r \in \mathbf{R}^{(p+2)N+1} \mid e^{-\langle c(\cdot), r \rangle} \in H^{\nu} \right\} \end{aligned}$$

R^{ν} often convex; \leq often replaces $=$
 \implies convex problem

Estimator **unique** under additional assumptions

Outline

- ▶ Density estimation as a stochastic program
- ▶ Epi-splines: pliable approximation tools
- ▶ **Consistency and asymptotics**
- ▶ Fusion of hard and soft information
- ▶ Numerical examples

Consistency

Kullback-Leibler projection of density h on $\text{e-spl}^p(m)$ is the set

$$\mathcal{P}_{p,m}(h) = \underset{s \in \text{e-spl}^p(m)}{\text{argmin}} \quad d_{KL}(h || e^{-s}) \text{ s.t. } \int_{m_0}^{m_N} e^{-s(x)} dx = 1$$

$$\mathcal{P}_{p,m}^S(h) = \text{KL-projection relative to } S \subset \text{e-spl}^p(m)$$

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$\mathcal{P}_{p,m}^S(h)$ = KL-projection **relative** to $S \subset \text{e-spl}^p(m)$

$$P_{p,m}^\nu : s^\nu \in \underset{s \in S^\nu}{\operatorname{argmin}} \frac{1}{\nu} \sum_{i=1}^{\nu} s(X^i) \text{ s.t. } \int_{m_0}^{m_N} e^{-s(x)} dx = 1$$

$$S^\nu = \{s \in \text{e-spl}^p(m) \mid e^{-s} \in H^\nu\}$$

Consistency (cont.)

True density $h^0 = e^{-s^0}$, with $s^0 = \langle c(\cdot), r^0 \rangle \in \text{e-spl}^p(m)$

Independent sample from h^0

$\{s^\nu\}_{\nu=1}^\infty$ sequence of optimal solutions of $P_{p,m}^\nu$, with $\{r^\nu\}_{\nu=1}^\infty$

Consistency (cont.)

True density $h^0 = e^{-s^0}$, with $s^0 = \langle c(\cdot), r^0 \rangle \in \text{e-spl}^p(m)$

Independent sample from h^0

$\{s^\nu\}_{\nu=1}^\infty$ sequence of optimal solutions of $P_{p,m}^\nu$, with $\{r^\nu\}_{\nu=1}^\infty$

If $\lim R^\nu$ exists almost surely and is deterministic, then every accumulation point r^∞ of $\{r^\nu\}_{\nu=1}^\infty$ satisfies

$$\langle c(\cdot), r^\infty \rangle \in \mathcal{P}_{p,m}^{S^\infty}(h^0) \text{ almost surely,}$$

where $S^\infty = \{s \in \text{e-spl}^p(m) \mid s = \langle c(\cdot), r \rangle, r \in \lim R^\nu\}$

Consistency (cont.)

Regardless of whether R^ν has a limit, if there exists $\{\hat{r}^\nu\}_{\nu=1}^\infty$, $\hat{r}^\nu \in R^\nu$, such that $\hat{r}^\nu \rightarrow r^0$ a.s., then a.s.:

- (i) $\langle c(\cdot), r^\infty \rangle \in \mathcal{P}_{p,m}(h^0)$
- (ii) $r_{\text{ess}}^\infty = r_{\text{ess}}^0$ ('essential' part: $r^0 = (r_{\text{mesh}}^0, r_{\text{ess}}^0)$)
- (iii) If $r^\nu \rightarrow^K r^\infty$ along a subsequence K , then

$$\langle c(\cdot), r^\nu \rangle \rightarrow^K s^0 \text{ and } e^{-\langle c(\cdot), r^\nu \rangle} \rightarrow^K h^0$$

uniformly on $[m_0, m_N]$, possibly except on m

Proof of consistency

- ▶ Let X^0 have density h^0 .
- ▶ Since $X^0 \in [m_0, m_N]$ almost surely, $c(X^0)$ is a random vector with finite moments
- ▶ Law of large number $(1/\nu) \sum_{i=1}^{\nu} c(X^i) \rightarrow E\{c(X^0)\}$ a.s.
- ▶ Epi-convergence of (effective) objective functions follow

Stability of Kullback-Leibler projection

Densities h^ν, h^0 on $[l, u]$ satisfy $dl_{\text{hypo}}(h^\nu, h^0) \rightarrow 0$

If r^ν is such that

$$\langle c(\cdot), r^\nu \rangle \in \mathcal{P}_{p,m}(h^\nu) \text{ for } m = \{m_k\}_{k=0}^N, m_0 = l, m_N = u,$$

then every accumulation point of $\{r^\nu\}_{\nu=1}^\infty$ is the epi-spline parameter of some $s^0 \in \mathcal{P}_{p,m}(h^0)$

Connections between modes of convergence

Densities $h^\nu, h^0 \in \mathbf{x}\text{-spl}^p(m)$, with $h^\nu = e^{-\langle c(\cdot), r^\nu \rangle}$, $h^0 = e^{-\langle c(\cdot), r^0 \rangle}$

Then,

$$r^\nu \rightarrow r^0 \implies d_{KL}(h^0 || h^\nu) \rightarrow 0 \iff d_{KL}(h^\nu || h^0) \rightarrow 0 \implies r_{\text{ess}}^\nu \rightarrow r_{\text{ess}}^0$$

Asymptotic normality

True density $h^0 = e^{-s^0} \in \text{x-spl}^p(m)$, $s^0 = \langle c(\cdot), r^0 \rangle$

r^0 in the interior of $\liminf R^\nu$ a.s.

Independent sample from h^0

$\{s^\nu\}_{\nu=1}^\infty$ optimal solutions of $P_{p,m}^\nu$, with $\{r^\nu\}_{\nu=1}^\infty$, $h^\nu = e^{-\langle c(\cdot), r^\nu \rangle}$

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Independent sample from h^0

$\{s^\nu\}_{\nu=1}^\infty$ optimal solutions of $P_{p,m}^\nu$, with $\{r^\nu\}_{\nu=1}^\infty$, $h^\nu = e^{-\langle c(\cdot), r^\nu \rangle}$

Then:

$$\nu^{1/2}(r_{\text{ess}}^\nu - r_{\text{ess}}^0) \rightarrow^d \mathcal{N}(0, \Sigma(r_{\text{ess}}^0))$$

$$\nu^{1/2}(h^\nu(x) - h^0(x)) \rightarrow^d \mathcal{N}(0, \Sigma_x(r_{\text{ess}}^0)), \quad x \in (m_{k-1}, m_k), \quad k = 1, \dots, N$$

Moment estimator $\mu_j^\nu = \int_{m_0}^{m_N} x^j e^{-\langle c(x), r^\nu \rangle} dx$ satisfies

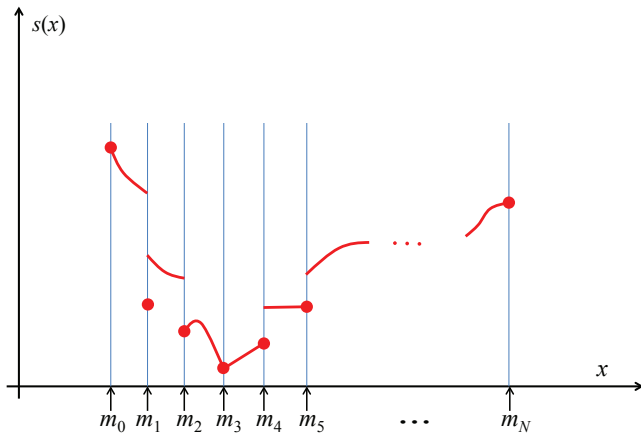
$$\nu^{1/2}(\mu_j^\nu - \mu_j^0) \rightarrow^d \mathcal{N}(0, \langle w, \Sigma(r_{\text{ess}}^0) w \rangle)$$

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Formulation of soft information

Easy to ensure bounds on domain, continuity, smoothness, monotonicity



Continuity

Epi-spline parameter

$r =$

$(s_0, \dots, s_N, a_{1,0}, a_{1,1}, \dots, a_{1,p}, a_{2,0}, a_{2,1}, \dots, a_{2,p}, \dots, a_{N,0}, a_{N,1}, \dots, a_{N,p})$

$$s_{k-1} = a_{k,0}, \quad s_k = \sum_{i=0}^p a_{k,i} (m_k - m_{k-1})^i, \quad k = 1, 2, \dots, N$$

Kullback-Leibler constraint

Recall: **Kullback-Leibler** divergence from density h to density g

$$d_{KL}(h||g) = \int_{-\infty}^{\infty} h(x) \log \frac{h(x)}{g(x)} dx$$

If $s \in \text{e-spl}^p(m)$ and r its epi-spline parameter, then

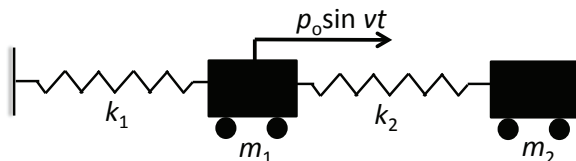
$$d_{KL}(h||e^{-s}) = \left\langle \int_{m_0}^{m_N} c(x)h(x)dx, r \right\rangle + \int_{-\infty}^{\infty} (\log h(x))h(x)dx,$$

So $\kappa_1 \leq d_{KL}(h||e^{-s}) \leq \kappa_2$ are **linear constraints**

Outline

- ▶ Density estimation as a stochastic program
- ▶ Epi-splines: pliable approximation tools
- ▶ Consistency and asymptotics
- ▶ Fusion of hard and soft information
- ▶ Numerical examples

Example: 2-dof dynamical system



$$m_1 \ddot{u}_1(t) + (k_1 + k_2)u_1(t) - k_2 u_2(t) = p_o \sin vt$$

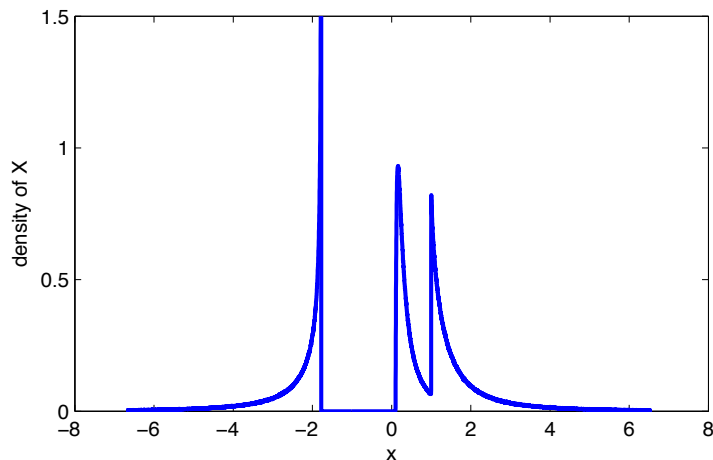
$$m_2 \ddot{u}_2(t) - k_2 u_1(t) + k_2 u_2(t) = 0$$

For choices of k_i , m_i , steady-state displacement at node 2:

$$u_2(t) = u_{2o} \sin vt \text{ with amplitude } u_{2o} = \frac{1}{(1 - v^2)(1 - v^2/4)}$$

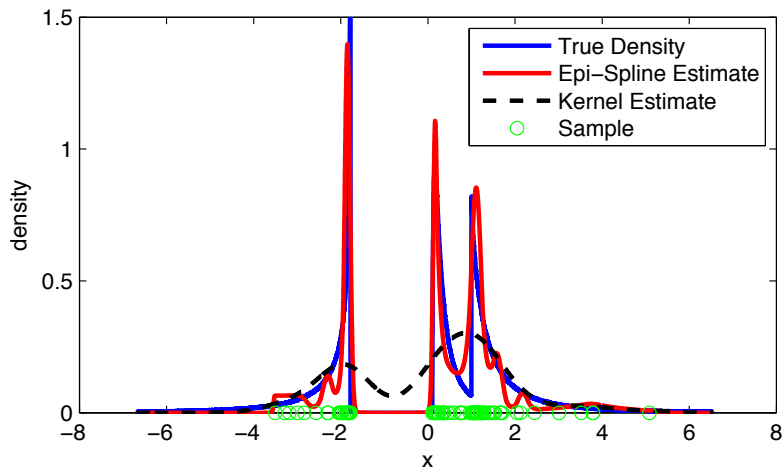
Example: Density of response amplitude

V mix of beta densities gives density for amplitude X :



Example: Density of response amplitude (cont.)

Sample size 100; continuously differentiable; “unimodal” tails



Gradient information

Gradient information for bijective $G : \mathcal{R} \rightarrow \mathcal{R}$

Recall: If $X = G(V)$, then

$$h_X(x) = h_V(G^{-1}(x)) / |G'(G^{-1}(x))|$$

Present context *without* a bijection and data $x^i = G(v^i)$, $G'(v^i)$:

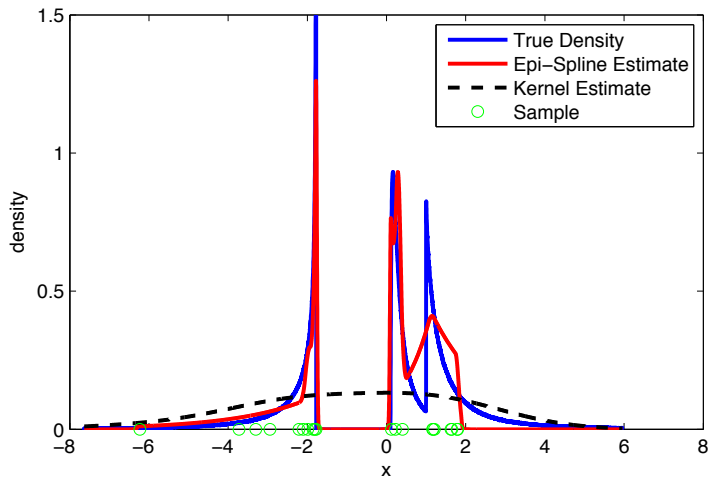
$$h^\nu(x^i) = e^{-\langle c(x^i), r \rangle} \geq \frac{h_V(v^i)}{|G'(v^i)|}$$

$$\langle c(x^i), r \rangle \leq -\log \frac{h_V(v^i)}{|G'(v^i)|}$$

Value of pdf **bounded from below** at x^i

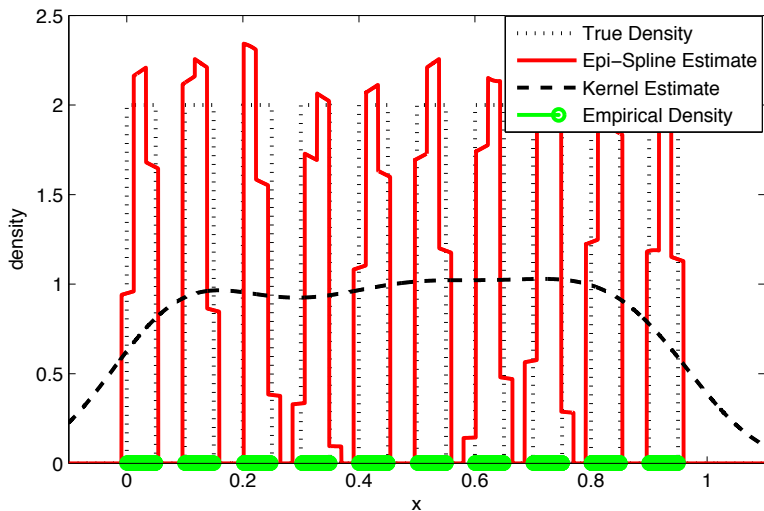
Back to example

Sample size 20; gradient information



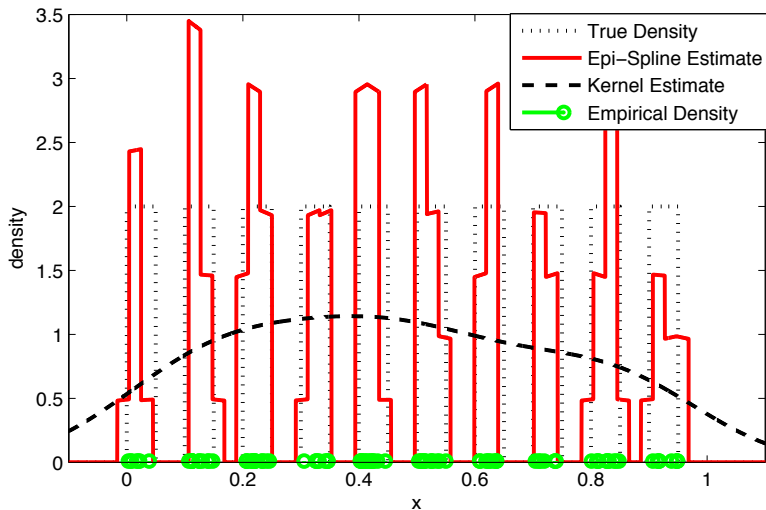
Example: Uniform mixture density

sample size 1000; lsc



Example: Uniform mixture density (cont.)

sample size just 100; lsc



Summary

- ▶ Density estimation problems as stochastic programs
- ▶ Exponential epi-splines offer a tractable class of density estimators
- ▶ Incorporate soft information by means of constraints
- ▶ Extensions to response surface, regression curve, multivariate density estimation, and many other curve fitting problems

References

- ▶ Royset & Wets, “Nonparametric density estimation via exponential epi-splines: fusion of soft and hard information”
- ▶ Royset & Wets, “Epi-splines and exponential epi-splines: Pliable approximation tools”
- ▶ Singham, Royset, & Wets, “Density estimation of simulation output using exponential epi-splines,” *Proc. WSC*, 2013
- ▶ Royset, Sukumar, & Wets “Uncertainty quantification using exponential epi-splines,” *Proc. ICOSAR*, 2013
- ▶ More examples: <https://www.math.ucdavis.edu/~prop01/>
- ▶ Matlab implementations available